

- $E_n = \left(n + \frac{1}{2}\right) \hbar \omega$
- $a^\dagger \psi_n = \sqrt{n+1} \psi_{n+1} \quad a \psi_n = \sqrt{n} \psi_{n-1}$
- $\psi_n = \frac{1}{\sqrt{n!}} (a^\dagger)^n \psi_0$
- $a = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i}{m\omega} \hat{p} \right), \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i}{m\omega} \hat{p} \right)$
- $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger), \quad \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}} (a^\dagger - a)$

4 The Free Particle

- $V(x) = 0$ everywhere
- Wave packet: $\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m} t)} dk$
- $\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x, 0) e^{-ikx} dx$
- $k \equiv \pm \frac{\sqrt{2mE}}{\hbar}, \quad \text{with } \begin{cases} k > 0 & \Rightarrow \text{traveling to the right} \\ k < 0 & \Rightarrow \text{traveling to the left} \end{cases}$
- Group velocity: $v_{group} = \frac{d\omega}{dk}$
- Phase velocity: $v_{phase} = \frac{\omega}{k}$

5 The Hydrogen Atom

- $E_n = \frac{-13.6 \text{ eV}}{n^2}$
- $\psi_{100}(r, \theta, \phi) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}, \quad a = 0.53 \times 10^{-10} \text{ m}$
- Selection rules for transitions:
 - $\Delta l = \pm 1, \quad \Delta m = \pm 1, 0$

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Thomas S. Hofer, Sam P. de Visser



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Chemistry that highlight novel approaches as well as advanced applications of QM MM method to a broad variety of targets In total 2 review articles and 10 original research contributions from 48 authors are presented covering 12 different countries on four continents The range of research questions addressed by the individual contributions provide a lucid overview on the versatility of the QM MM method and demonstrate the general applicability and accuracy that can be achieved for different problems in chemical sciences Together with the development of improved algorithms to enhance the capabilities of quantum chemical methods and the continuous advancement in the capacities of computational resources it can be expected that the impact of QM MM methods in chemical sciences will be further increased already in the near future

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